Effective properties of random composites

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Abstract

We propose a new concept for effective properties of composites with uncertain spatial arrangements of constitutive materials and within-material properties. Rather than replacing a heterogeneous property with a constant effective parameter, we seek to preserve composite's internal macro structure. This general concept is used to derive an effective conductivity of composite porous media, when both material's geometry and conductivities within each material are uncertain. Our analysis uses a random domain decomposition to explicitly account for the separate effects of material and geometric uncertainty on ensemble moments of pressure and flux. We present a general expression for the effective (apparent) conductivity of such media and analyze it in detail for one- and two-dimensional steady flows in bounded random media composed of two materials with highly contrasting conductivities.

Keywords: composite media, random fields, moment equations, effective, equivalent

1 Introduction

Effective (upscaled) parameters have proved to be a useful tool for modeling heterogeneous systems. Such models often require assigning system parameters to large grid blocks, while experimental data are usually available at a much smaller scale. These parameters can be obtained through either deterministic approaches, such as homogenization and inverse modeling, or stochastic averaging – the approach we pursue here. A plethora of approaches used to obtain effective (apparent) parameters for composites is reviewed by Milton (2002). These and other methods seek to replace a heterogeneous system with a homogeneous system that preserves some global properties. Consider, for example, diffusion in a medium composed of several heterogeneous materials whose spatial arrangement is uncertain. Standard upscaling or homogenization techniques substitute the effective diffusion coefficient K_{eff} for the space varying diffusion coefficient $K(\boldsymbol{x})$ in a way that preserves a global mass flux induced by a global gradient of substance. While often useful, such effective parameters fail to predict important characteristics of the system behavior, e.g. the existence of preferential flow paths in porous media. In fact, rapid advances in noninvasive data collection techniques, such as magnetic resonance imaging and computerized axial tomography, make it unnecessary to homogenize a system in ways that ignore the internal composition of a material. What is required is to derive effective parameters that incorporate uncertainties in both the material properties and internal boundaries. This paper takes a first step in this direction.

Stochastic approaches to upscaling are grounded in the fact that in realistic settings the system parameters are deduced from measurements at selected locations and depth intervals, where their values depend on the scale and mode of measurement. Quite often, the measurement support is uncertain and data are corrupted by experimental and interpretative errors. Estimating the parameters at points where measurements are not available entails additional errors. Treating the system parameters as random fields provides a natural framework for dealing with these errors and uncertainties. Within this framework a system parameter $K(\boldsymbol{x})$ is characterized by a joint (multivariate) probability density function or, equivalently, its joint ensemble moments. Thus, $K(\boldsymbol{x})$ varies not only across the real space coordinates $\boldsymbol{x}$, but also in probability space (this variation may be represented by another coordinate $\boldsymbol{\xi}$, which, for simplicity of notation, is usually suppressed). Whereas spatial moments of K are obtained by sampling $K(\boldsymbol{x})$ in real space (across $\boldsymbol{x}$), its ensemble moments are defined in terms of samples collected in probability space (across $\boldsymbol{\xi}$).

Randomness of the system parameters renders partial differential equations (PDEs), which govern dynamics of the system states, stochastic. The effective (equivalent, apparent) parameters are then defined as coefficients in the ensemble averaged stochastic PDEs. Consider, for example, Darcy's law, $\boldsymbol{q} = -K\nabla h$, which postulates a linear relationship between the mass flux $\boldsymbol{q}(\boldsymbol{x})$ and the pressure gradient $\nabla h(\boldsymbol{x})$ in porous media. The apparent conductivity $K_{\text{app}}(\boldsymbol{x})$ is defined as a coefficient of proportionality in the ensemble averaged Darcy's law, $\langle \boldsymbol{q} \rangle = -K_{\text{app}} \nabla \langle h \rangle$. The term "apparent" was introduced by Dagan (2001) to emphasize that the effective parameters thus defined are local properties, which depend not only on material properties, but on the external forces (e.g. boundary conditions) as well.

To derive the effective parameters that preserve internal structure of a composite, we employ the random domain decomposition approach (Winter and Tartakovsky, 2000, 2002). It allows us to deal with uncertainty in both spatial arrangement of the composite materials and their parameters. While an approach we propose promises to be applicable to a wide variety of physical systems, in this paper we focus on deriving the effective conductivity of porous media composed of multiple facies. The main results of our study are formulated in Sections 3 and 4, where we provide a general expression for the effective conductivity of a composite and analyze it, both analytically and numerically, for one- and two-dimensional flow configurations.

2 Problem Formulation

Consider steady-state saturated flow in a flow domain $\Omega = \Omega_1 \cup \Omega_2$, which is composed of two disjoint sub-domains, Ω_1 and Ω_2, separated by a contact surface $\Gamma_{12} = \Omega_1 \cap \Omega_2$. It is described by Darcy's law and the mass conservation,

$$\boldsymbol{q} = -K\nabla h, \qquad -\nabla \cdot \boldsymbol{q} + f = 0, \tag{1}$$

where f is a (generally random) forcing term. We allow for the presence of both the Dirichlet, Γ_D, and Neumann, Γ_N, boundaries, on which the respective boundary conditions hold

$$h(\boldsymbol{x}) = H(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Gamma_D, \tag{2a}$$

$$K(\boldsymbol{x})\nabla h(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) = Q(\boldsymbol{x}), \qquad \boldsymbol{x} \in G_N, \tag{2b}$$

where $\boldsymbol{n}$ is the unit vector normal to the boundary.

Let the random hydraulic conductivity field belong to two distinct populations,

$$K(\boldsymbol{x}) = \begin{cases} K_1(\boldsymbol{x}), & \boldsymbol{x} \in \Omega_1, \\ K_2(\boldsymbol{x}), & \boldsymbol{x} \in \Omega_2. \end{cases} \tag{3}$$

Then the flow equation can be rewritten as

$$\nabla \cdot K_i \nabla h + f = 0, \qquad \boldsymbol{x} \in \Omega_i. \tag{4}$$

The boundary conditions (2) are now supplemented by the continuity conditions on the random interface, Γ_{12},

$$h(\boldsymbol{x}^-) = h(\boldsymbol{x}^+) \tag{5a}$$

$$K(\boldsymbol{x}^-)\nabla h(\boldsymbol{x}^-) \cdot \boldsymbol{n}(\boldsymbol{x}^-) = K(\boldsymbol{x}^+)\nabla h(\boldsymbol{x}^+) \cdot \boldsymbol{n}(\boldsymbol{x}^+). \tag{5b}$$

Here the superscripts $^-$ and $^+$ indicate the limits as $\boldsymbol{x} \to \Gamma_{12}$ from Ω_1 and Ω_2, respectively.

In this formulation, the randomness of $K(\boldsymbol{x})$ stems from the two factors: a small scale, within material uncertainty in $K_i(\boldsymbol{x})$ and a large scale uncertainty in the spatial arrangement of Ω_i or, equivalently, in the boundary Γ_{12}. Hence $p_K(k)$, the probability density function of K, is replaced with $p_K(k, \Gamma_{12}) = p_K(k|\Gamma_{12})p_\Gamma(\gamma)$, a joint probability density function. While, for highly contrasting composites, $p_K(k)$ is multi-modal with large variance σ_K^2, a conditional distribution $p_K(k|\Gamma_{12})$ – that represents conductivity's fluctuations within each material Ω_i – is likely to be uni-modal with small variances $\sigma_{K_i}^2$. This is important because closure approximations associated with the stochastic (conditional) averaging of the flow equation (4) are carried out within each sub-domain Ω_i separately.

3 Apparent Conductivity

The mean Darcy's law,

$$\langle \boldsymbol{q}(\boldsymbol{x}) \rangle = -\langle K_i(\boldsymbol{x}) \rangle \nabla \langle h(\boldsymbol{x}) \rangle + \boldsymbol{r}_i(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega_i, \tag{6}$$

is derived by applying Reynolds decomposition to represent random fields $\mathcal{R} = \langle \mathcal{R} \rangle + \mathcal{R}'$ as the sum of their ensemble means $\langle \mathcal{R} \rangle$ and zero-mean fluctuations $\mathcal{R}'$ and averaging in the probability space. In (6), $\langle K_i(\boldsymbol{x}) \rangle$ denotes the (ensemble) mean conductivity of the i-th material, and $\boldsymbol{r}_i = -\nabla \langle K_i' \nabla h' \rangle$ is the residual flux, representing the cross-covariance between the pressure gradient and conductivity fluctuations. The residual flux, conditioned on Γ_{12}, can be found as a solution of an integral equation (Winter and Tartakovsky, 2000)

$$\boldsymbol{r}_i(\boldsymbol{x}|\Gamma) = \int_{\Omega_i} \boldsymbol{a}_i(\boldsymbol{y}, \boldsymbol{x}) \nabla \langle h(\boldsymbol{y}) \rangle d\boldsymbol{y} + \int_{\Omega_i} \boldsymbol{b}_i(\boldsymbol{y}, \boldsymbol{x}) \boldsymbol{r}_i(\boldsymbol{y}) d\boldsymbol{y} \tag{7}$$

where $\boldsymbol{a}_i$ and $\boldsymbol{b}_i$ are symmetric positive-semidefinite and non-symmetric dyadic, respectively. The residual flux is then computed by evaluating the integral $\boldsymbol{r}_i(\boldsymbol{x}) = \int \boldsymbol{r}_i(\boldsymbol{x}|\Gamma) dP_\Gamma(\gamma)$. It follows from (6) and (7) that the mean Darcy's flux $\langle \boldsymbol{q}(\boldsymbol{x}) \rangle$ is nonlocal, i.e., depends on the mean head gradient $\nabla \langle h \rangle$ at points other than $\boldsymbol{x}$. Hence the effective (apparent) conductivity does not generally exist.

Assume that both the mean pressure gradient and the residual flux vary slowly in space. Then (7) can be localized, leading to an approximate expression (Tartakovsky et al., 2002)

$$\boldsymbol{r}_i(\boldsymbol{x}) \approx \boldsymbol{A}_i(\boldsymbol{x})\nabla\langle h(\boldsymbol{x})\rangle + \boldsymbol{B}_i(\boldsymbol{x})\boldsymbol{r}_i(\boldsymbol{x}) \tag{8}$$

where

$$\boldsymbol{A}_i(\boldsymbol{x}|\Gamma) = \int_{\Omega_i} \boldsymbol{a}_i(\boldsymbol{y},\boldsymbol{x})d\boldsymbol{y} \qquad \text{and} \qquad \boldsymbol{B}_i(\boldsymbol{x}|\Gamma) = \int_{\Omega_i} \boldsymbol{b}_i(\boldsymbol{y},\boldsymbol{x})d\boldsymbol{y}. \tag{9}$$

This gives an approximate (localized) form of the mean Darcy's law

$$\langle \boldsymbol{q}(\boldsymbol{x})\rangle = -\boldsymbol{K}_{\mathrm{app}_i}(\boldsymbol{x})\nabla\langle h(\boldsymbol{x})\rangle, \qquad \boldsymbol{x} \in \Omega_i. \tag{10}$$

The spatially varying apparent conductivity tensor is given by

$$\boldsymbol{K}_{\mathrm{app}_i}(\boldsymbol{x}) = \langle K_i(\boldsymbol{x})\rangle \boldsymbol{I} + \boldsymbol{k}_i(\boldsymbol{x}) \tag{11}$$

where

$$\boldsymbol{k}_i(\boldsymbol{x}) = \big[\boldsymbol{I} - \boldsymbol{B}_i(\boldsymbol{x})\big]^{-1}\boldsymbol{A}_i(\boldsymbol{x}) \tag{12}$$

and $\boldsymbol{I}$ is the identity tensor. Evaluation of the apparent conductivity requires a closure approximation of the tensors $\boldsymbol{a}$ and $\boldsymbol{b}$ in (9). One such closure is ontained through a perturbation expansion in σ_Y^2, the variance of log-hydraulic conductivity $Y = \ln K$. The first-order (in $\sigma_{Y_i}^2$) approximation of the conditional apparent conductivity tensor is

$$\boldsymbol{K}_{\mathrm{app}_i}^{[1]}(\boldsymbol{x}|\Gamma) = K_{g_i}\left(1 + \frac{\sigma_{Y_i}^2}{2}\right)\boldsymbol{I} - K_{g_i}\int_{\Omega_i} \sigma_{Y_i}^2 K_{g_i}\rho_{Y_{ii}}(\boldsymbol{y},\boldsymbol{x})\nabla_{\boldsymbol{y}}\nabla_{\boldsymbol{x}}^T G(\boldsymbol{y},\boldsymbol{x})d\boldsymbol{y} \tag{13}$$

Here $K_{g_i}(\boldsymbol{x})$ is the geometric mean of the local conductivity in the ith material, $\rho_{Y_{ii}}$ is the two-point correlation function of Y for $\boldsymbol{x},\boldsymbol{y} \in \Omega_i$, and G_i is the conditional mean Green's function for (4) wherein the random fields K_i are replaced with their geometric means K_{g_i}. It is important to note that (13) represents the conditional apparent conductivity, since it corresponds to a realization of the random sub-domains Ω_i. The final step in obtaining the apparent conductivity consists of the ensemble averaging in the probability space of the internal geometries Ω_i.

The perturbation approximation in (13) is carried out in terms of the variances within the materials, $\sigma_{Y_i}^2$, which are small in most natural formations. However, if they are not small enough for (13) to remain accurate, one can generalize this expression by means of the Landau-Matheron conjecture (e.g., Paleologos et al., 1996).

4 Computational Examples

To analyze our general expression for the apparent conductivity of composite media in detail, we consider one- and two-dimensional flows in layered media. The one-dimensional example is amenable to analytical analysis, while the two-dimensional example relies on numerical evaluation of the Green's function and quadratures in (13).

4.1 One-Dimensional Flow

Consider the one-dimensional version of (4) with $f \equiv 0$, which is defined on the interval $x \in \Omega = (0,1)$. The boundary conditions are

$$K\frac{dh}{dx} = -Q \qquad \text{for} \qquad x = 0 \tag{14a}$$

and

$$h(x) = 0 \qquad \text{for} \qquad x = 1. \tag{14b}$$

The domain Ω is composed of two materials $\Omega_1 = [0,\beta]$ and $\Omega_2 = (\beta,1]$ joint at the point $x = \beta$. The continuity conditions at $x = \beta$ are

$$h(\beta^-) = h(\beta^+) \qquad \text{for} \qquad K_1(\beta^-)\frac{dh(x=\beta^-)}{dx} = K_2(\beta^+)\frac{dh(x=\beta^+)}{dx}. \tag{15}$$

The sub-domains Ω_1 and Ω_2 are characterized by the random conductivity fields K_1 and K_2, respectively. These are assumed to be log-normal, statistically homogeneous, and uncorrelated with each other. The fields $Y_i = \ln K_i$ are fully described by their geometric means $K_{g_i} = \exp(\langle Y_i \rangle)$, variances $\sigma^2_{Y_i}$, and correlation functions $\rho_{Y_i}(y,x)$.

The contact point β is assumed to be truncated Gaussian, with the mean $\langle\beta\rangle$ and the variance σ^2_β, so that its probability density function is

$$p(\beta) = \frac{1}{\mathcal{W}}\exp\left[-\frac{1}{2}\left(\frac{\beta - \langle\beta\rangle}{\sigma_\beta}\right)^2\right], \qquad \mathcal{W}(\langle\beta\rangle,\sigma_\beta) = \int_0^1 \exp\left[-\frac{1}{2}\left(\frac{\beta - \langle\beta\rangle}{\sigma_\beta}\right)^2\right] d\beta. \tag{16}$$

4.1.1 First-order approximation

It is easy to verify that the conditional mean Green's function, $G(y,x)$, is given by

$$G(y, x \le \beta) = \begin{cases} \frac{x-y}{K_{g1}}\mathcal{H}(y-x) + \frac{\beta - x}{K_{g1}} + \frac{1-\beta}{K_{g2}}, & 0 < y \le \beta, \\ \frac{1-y}{K_{g2}}, & \beta < y < 1 \end{cases} \tag{17a}$$

and

$$G(y, x > \beta) = \begin{cases} \frac{1-x}{K_{g2}}, & 0 < y \le \beta, \\ \frac{x-y}{K_{g2}}\mathcal{H}(y-x) + \frac{1-x}{K_{g2}}, & \beta < y < 1. \end{cases} \tag{17b}$$

where $\mathcal{H}(z)$ is the Heaviside function. Substituting (17) into the one-dimensional version of (13) yields, for any $\rho(y,x)$,

$$K^{[1]}_{\mathrm{app}}(x|\beta) = K_{g1}\left(1 - \frac{\sigma^2_{Y_1}}{2}\right)\mathcal{H}(\beta - x) + K_{g2}\left(1 - \frac{\sigma^2_{Y_2}}{2}\right)\mathcal{H}(x-\beta). \tag{18}$$

To ascertain the accuracy of the perturbation approximation of the conditional apparent conductivity, we derive in the next section the corresponding exact expression.

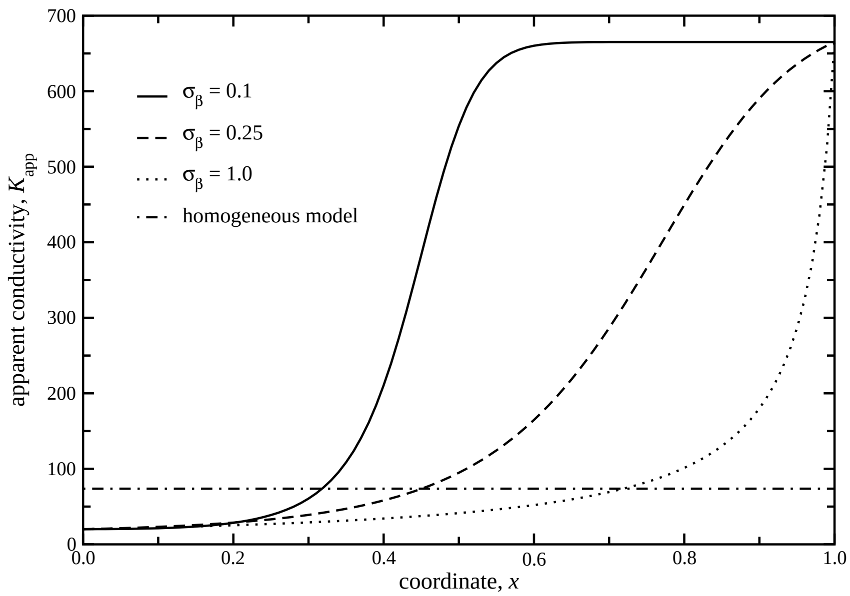

Figure 1: Apparent conductivity, K_{app}, for the one-dimensional random composite with uncertain internal geometry, β, and material conductivities, K_1 and K_2.

4.1.2 Exact solution

Integrating the flow equation once and taking the conditional mean yields

$$\frac{d\langle h\rangle}{dx} = -Q\left[\frac{\mathcal{H}(\beta - x)}{K_{h_1}} + \frac{\mathcal{H}(x-\beta)}{K_{h_2}}\right] \tag{19}$$

where $K_{h_i} = K_{g_i}\exp(-\sigma^2_{Y_i}/2)$ is the harmonic mean of K_i. Thus the conditional apparent conductivity is given by

$$K^{-1}_{\text{app}}(x|\beta) = \frac{\mathcal{H}(\beta - x)}{K_{h_1}} + \frac{\mathcal{H}(x-\beta)}{K_{h_2}}. \tag{20}$$

Comparing (18) and (20), while recalling the definition of the harmonic mean, shows that (18) is indeed the first-order approximation of the exact expression (20). The approximation (18) remains accurate as long as both $\sigma^2_{Y_i} < 2$.

It is important to contrast our expression for the (conditional) apparent conductivity with the traditional apparent conductivity that effectively homogenizes the medium. One can easily verify that the latter is given by the weighted sum of the sub-domains' harmonic means,

$$K^{-1}_{\text{hom}} = \frac{\beta}{K_{h_1}} + \frac{1-\beta}{K_{h_2}}. \tag{21}$$

Of course, the traditional definition of apparent conductivity is constant in space.

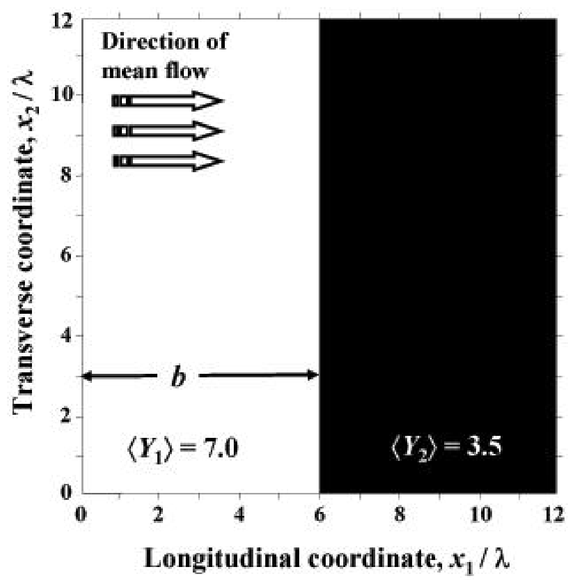

Figure 2: Flow domain geometry.

The final step in obtaining the apparent conductivity is to average the conditional apparent conductivity (20), or its first-order approximation (18), in the probability space of β. For β whose probability density function is given by (16), the apparent conductivity takes the form

$$K_{\text{app}}^{-1}(x) = \frac{\operatorname{erf}(u) - \operatorname{erf}(u_0)}{\operatorname{erf}(u_1) - \operatorname{erf}(u_0)} \left[\frac{1}{K_{h_1}} - \frac{1}{K_{h_2}} \right] + \frac{1}{K_{h_1}}. \tag{22}$$

where

$$u = \frac{x - \langle \beta \rangle}{\sqrt{2}\,\sigma_\beta}, \qquad u_0 = -\frac{\langle \beta \rangle}{\sqrt{2}\,\sigma_\beta}, \qquad u_1 = \frac{1 - \langle \beta \rangle}{\sqrt{2}\,\sigma_\beta}. \tag{23}$$

Figure 1 shows spatial variations of the apparent conductivity $K_{\text{app}}(x)$ for $\langle Y_1 \rangle = 3.5$, $\langle Y_2 \rangle = 7.0$, $\sigma_{Y_1}^2 = \sigma_{Y_2}^2 = 1$, $\langle \beta \rangle = 0.25$ and several values of σ_β. These are contrasted with the constant K_{app} corresponding to the homogeneous model (21). As can be seen from Fig. 1, and follows directly from (22), the apparent conductivity $K_{\text{app}}(x)$ is given by the harmonic means K_{h_1} or K_{h_2}, when x is deep withing sub-domains Ω_1 or Ω_2. A width of the transitional zone between these two harmonic means increases with uncertainty in β, i.e., with σ_β. If β is known with certainty, i.e., $\sigma_\beta = 0$, $K_{\text{app}}(x)$ becomes a step function, and (22) reduces to (20).

4.2 Two-Dimensional Flow

Consider flow in a square domain composed of two materials separated by an uncertain boundary (Figure 2). The materials are characterized by the log conductivities $Y_i = \ln K_i$, which are treated as statistically homogeneous Gaussian random fields with the means $\langle Y_1 \rangle = 3.5$ and $\langle Y_2 \rangle = 7.0$, the variances $\sigma_{Y_1}^2 = \sigma_{Y_2}^2 = 1$ and the two-point exponential correlation functions ρ_{Y_i} of the unit correlation lengths $\lambda_{Y_1} = \lambda_{Y_2} = 1$. For simplicity, conductivities of different materials are taken to be uncorrelated. The random location, $x_1 = \beta$, of the internal boundary between the two materials is taken to be Gaussian, with the mean $\langle \beta \rangle = L/2$ and the variance σ_β^2, where L is the square size.

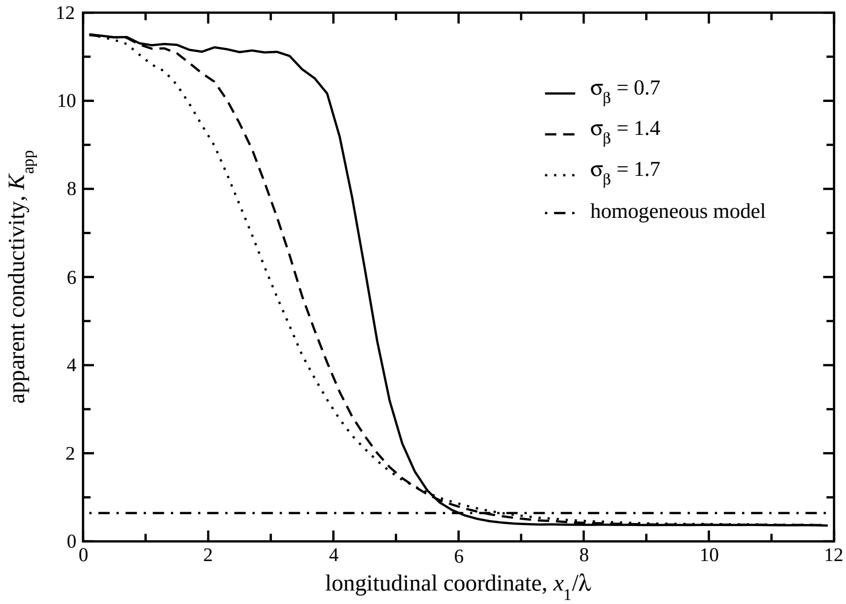

Figure 3: Horizontal cross-section $x_2 = L/2$ of the apparent conductivity, $K_{\rm app}$, for the two-dimensional random composite with uncertain internal boundary, $x_1 = \beta$, and material conductivities, K_1 and K_2.

Of course, the resulting conductivity field is statistically inhomogeneous, in that its mean, variance and correlation function are all space dependent.

The Dirichlet boundary conditions are prescribed on the vertical boundaries, $h(0, y) = H_a$ and $h(L, y) = H_b$, while the remaining two boundaries $(y = 0, L)$ are assumed to be impermeable. In the reported simulations, we set $H_a = 1.6$, $H_b = 1.0$, and $L = 12$.

The apparent conductivity $K_{\rm app}$ in (13) is obtained by evaluating numerically (i) the conditional mean Green's functions for each realization of β, (ii) quadratures in (13), and (iii) weighted averages of the conditional apparent conductivities, whose weights are determined from the distribution of β. Figure 3 shows a horizontal cross-section, $x_2 = L/2$, of $K_{\rm app}$ for several values of σ_β. The apparent conductivity of the two-dimensional composite exhibits the same general behavior as its one-dimensional counterpart.

5 Conclusions

We presented an expression for apparent (effective) conductivity of porous media composed of different materials (geologic facies) whose internal geometries and conductivities are uncertain. Our work leads to the following major conclusions:

1. Apparent (effective) conductivity of the composites should preserve their internal structure whenever possible. This is crucial for probabilistic analyses of system's critical behavior, e.g. the existence of preferential flow paths in natural porous media.

2. For steady-state flow in bounded heterogeneous composite media, we derived a general expression for the apparent conductivity by means of a perturbation expansion in the variances of materials' log-conductivities. Since the conductivity of each material is more uniform than that of the composite as a whole, this expression is more accurate and robust than its homogeneous counterpart.

3. The general perturbation expression for apparent conductivity is analyzed in detail for one- and two-dimensional steady flow in the bounded porous medium composed of two materials. Both materials' log-conductivities and the internal boundaries between the materials are assumed to be Gaussian. Apparent conductivity is given by the harmonic means of the corresponding conductivities of each material for points away from the internal boundary, and varies smoothly between these harmonic means within a transitional zone around the boundary. A width of the transitional zone increases with the degree of uncertainty about the internal boundary.

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